Isospin Lattice Gas Model and Nuclear-Matter Phase Diagram and Pressure-Volume Isotherms [1]

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ABSTRACT

We study a cubic lattice gas model for nuclear matter where each lattice site can be either occupied, by one proton or one neutron, or unoccupied. A nearest-neighbor interaction of the form $-\sum_{<ij>} J_{ij}\tau_{zi}\tau_{zj}$ is assumed. Our model is an isospin-1 Ising model, with τ_z = (1,0,-1) representing respectively (proton, vacancy, neutron). A kinetic-energy term has been included in our model. Under the Bragg-Williams mean field approximation our model exhibits the existence of a dense phase (liquid-like) and a rare phase (gas-like). The nuclear-matter p-v isotherms given by our model are discussed.

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It is believed that nuclear matter should exhibit a quark deconfinement phase transition at high temperatures ($k_BT \sim 200\ MeV$) and/or high densities ($\rho \sim 10\rho_0$), ρ_0 being the saturation density. At low temperatures ($k_BT \sim 15 - 20\ MeV$) and low densities ($\rho \sim \rho_0$) a liquid-gas phase transition of nuclear matter is expected to take place [1]. The underlying theoretical frameworks treating these two types of phase transitions have so far been very different.

For the former one generally uses lattice gauge QCD and Monte Carlo simulation [2]. The space-time structure here is a lattice. But for the latter, it has been a long tradition to employ standard many-body theories such as Hartree-Fock approximation [3, 4], real time Green's function method [5, 6], and ring-diagram summation method [7]. The space-time structure here is a continuous manifold. There appears to be a space-time disparity and one would like to ask the following questions: Is it necessary for nuclear systems to have so very different space-time geometry structures, namely a lattice and a continuum, in different energy and density domains? Can we set our theory on a unified footing so that a common lattice space-time manifold may be used to treat not only phase transitions in high-temperature and high-density regions but also those with low temperatures and low densities?

The above concern has motivated us to explore new schemes for studying nuclear matter in the low-temperature and -density regions. About forty years ago Lee and Yang [8] suggested a model of lattice gas where gas atoms are seated on a lattice. They mapped the problem of a lattice gas with one type of atom into an Ising model for spin half particles. They succeeded in describing a liquid-gas phase transition for atomic systems. We would like to generalize this model to nuclear matter which consists of two types of nucleons: proton and neutron. Here we consider a lattice with each site either being vacant or occupied by a proton or a neutron. One is tempted to associate Ising spin 1 to a proton, -1 to a neutron, and 0 to a vacancy. A preliminary account of our approach has been reported [9].

Nuclear forces may be understood based on one boson exchanges . The intermediate bosons include isoscalar bosons ($\omega, \sigma, ...$) and isovector bosons ($\pi, \rho, ...$). In this way, effective nucleon-nucleon(NN) interactions may be written in terms of a number of

standard components such as the spin-spin term $\sigma \cdot \sigma$, isospin-isospin term $\tau \cdot \tau$, and the spin-isospin term $\sigma \cdot \sigma \ \tau \cdot \tau$. If we average over the spin and spatial variables, we would obtain an effective interaction which depends on isospin only. The radial part of the NN interaction, to a reasonable approximation, can be represented by a nearest-neighbor square well potential with a repulsive hard core. Thus we are led to conjecture the following interaction hamiltonian for nuclear matter:

$$H_{int} = -\sum_{<ij>} J_{ij} \tau_{zi} \tau_{zj} \tag{1}$$

where

$$\tau_{zi} = \begin{cases} 1 & \text{for proton} \\ 0 & \text{for vacancy} \\ -1 & \text{for neutron.} \end{cases} \tag{2}$$

Note the above is a nearest-neighbor interaction, as indicated by the summation index $< ij >$, namely interaction exists only between adjacent neighbors. J_{ij} are interaction strength parameters. In fact we allow for two such parameters only; J_s for pp and nn interaction pairs and J_d for pn pairs. Clearly the above is a spin 1 Ising model [10, 11].

We rewrite eq.(1) as

$$H_{int} = -J_s(N_{++} + N_{--}) + J_d N_{+-} \tag{3}$$

where N_{++}, N_{--}... represent respectively the nearest neighbor pairs of proton-proton, neutron-neutron, etc. Note that in our model there is no interaction between vacancy and nucleon.

Now we proceed to calculate the thermodynamic quantities of our system. To facilitate the calculation, we introduce the following variables. Let N denote the total number of lattice sites, and N_+, N_-, N_0 denote respectively the number of proton, neutron and vacancy sites. We introduce

$$R = \frac{N_0}{N}, \ S = \frac{N_+ - N_-}{N}, \ N = N_+ + N_- + N_0 \tag{4}$$

where R and S represent the relative emptiness and proton-neutron asymmetry respectively. Note that in our model the nuclear-matter density ρ is proportional to (1-R).

The spin-1/2 lattice-gas models for atomic systems have been used with remarkable success in describing phase transitions. But they seem to have not, to our knowledge, been applied to calculate the pressure-volume isotherms. It has been suggested [12] that in order to describe these isotherms one needs to add the ideal-gas pressure to the lattice gas grand potential. The ideal gas pressure comes from the kinetic energy. Hence it would seem to be preferrable to include the the kinetic energy in the hamiltonian, from the beginning, rather than adding the ideal-gas pressure to the grand potential. The above consideration has motivated us to include a kinetic-energy term in our model, namely we employ a hamiltonian for the lattice gas of the form

$$H_{gas} = -J_s(N_{++} + N_{--}) + J_d N_{+-} + N\kappa(1-R)^{5/3} \tag{5}$$

where, guided by the Fermi gas model, we have assumed the kinetic energy per particle to be proportional to $\rho^{2/3}$. κ is a constant which we shall discuss later. The introduction of the kinetic-energy term is very important for our model, as we shall see soon.

As an initial investigation let us adopt the Bragg-Williams mean field approximation[12], namely

$$\frac{N_+^2}{N^2} \simeq \frac{N_{++}}{N\gamma/2},\ \frac{N_-^2}{N^2} \simeq \frac{N_{--}}{N\gamma/2},\ \frac{N_0^2}{N^2} \simeq \frac{N_{00}}{N\gamma/2} \tag{6}$$

where γ denotes the number of nearest neighbors of any given site, and $N\gamma/2$ is the total number of pairs. For three dimensional simple cubic lattice, $\gamma = 6$. From the constraints $\gamma N_+ = 2N_{++} + N_{+-} + N_{+0}$, $\gamma N_- = 2N_{--} + N_{+-} + N_{-0}$, $\gamma N_0 = 2N_{00} + N_{+0} + N_{-0}$ and $N = N_+ + N_- + N_0$, we obtain

$$N_{+-} = \gamma(N_+ + N_-) - (N_{++} + N_{--}) + N_{00} - \gamma N/2. \tag{7}$$

We can now rewrite our hamiltonian of eq.(5) as

$$H_{gas}(R,S,N) = -C_1 N S^2 - C_2 N(1-R)^2 + N\kappa(1-R)^{5/3} \tag{8}$$

where

$$C_1 = \frac{(J_s + J_d)\gamma}{4},\ C_2 = \frac{(J_s - J_d)\gamma}{4}. \tag{9}$$

The grand partition function of our system is

$$Q_G = \sum_{R,S} g(R,S,N) exp(-\bar{H}_{gas}/k_B T),$$

$$\bar{H}_{gas} = H_{gas}(R,S,N) - hNS - \lambda N(1-R) \tag{10}$$

The multiplicity factor [13] g is

$$g(R,S,N) = \frac{N!}{N_0! N_+! N_-!} = \frac{N!}{(NR)![N(1-R+S)/2]![N(1-R-S)/2]!}. \tag{11}$$

In $\bar{H}_{gas}$ we have included two Lagrange multipliers, h and λ. In our grand partition function, we sum over all possible R and S values. Thus we have neither a definite number of nucleons nor a definite proton-neutron assymmetry. The role of these Lagrange multipliers is to control the average values of R, denoted as $\bar{R}$, and of S, denoted as $\bar{S}$. For instance for symmetric nuclear matter we need $\bar{S}$=0, and this may be attained by varying h. Similarly, different $\bar{R}$ values may be obtained by varying λ.

Since our final goal is to study the thermodynamic limit ($N \to \infty$), we can replace the sum in the partition function Q_G by its most dominant term [13] (assuming the dominant term to be non-degenerate). Using Stirling's formula one obtains

$$\begin{aligned} -k_B T \ln Q_G &= -C_1 N S^2 - C_2 N (1-R)^2 - hNS \\ &\quad -\lambda N(1-R) + \kappa N (1-R)^{5/3} \\ &\quad + N k_B T [R \ln R + \frac{(1-R+S)}{2} \ln(1-R+S) \\ &\quad + \frac{(1-R-S)}{2} \ln(1-R-S) - (1-R)\ln 2] \end{aligned} \tag{12}$$

with the subsidiary extremum conditions

$$\frac{\partial(-k_B T \ln Q_G)}{\partial S} = \frac{N k_B T}{2} \ln \frac{1-R+S}{1-R-S} - [2C_1 S + h] N = 0, \tag{13}$$

$$\frac{\partial(-k_BT\ln Q_G)}{\partial R} = \frac{Nk_BT}{2}\ln\frac{4R^2}{(1-R)^2-S^2} + 2NC_2(1-R)$$

$$- \frac{5}{3}\kappa N(1-R)^{2/3} + \lambda = 0. \tag{14}$$

It is seen that $h = 0$ and $S = 0$ is a special solution which represents a symmetric nuclear matter. In this case eq.(13) becomes an identity and eq.(14) reduces to

$$k_BT\ln\frac{2R}{1-R} + 2C_2(1-R) - \frac{5}{3}\kappa(1-R)^{2/3} + \lambda = 0. \tag{15}$$

The analysis of this equation gives us the most important results of our present paper. It shows that below a certain temperature T_c we have two phases, one is dense (liquid-like) and the other is rare (gas-like). Above this temperature there is only one phase. The existence of a liquid-gas phase transition together with the determination of its phase diagram on the basis of a simple model that assumes only a phenomenological two body, nearest-neighbor interaction is quite remarkable. It seems to call for serious attention and further study.

Let us consider the λ=0 case first. In this case we rewrite eq.(15) as

$$\chi(R,T) = f(R) - g(R,T) = 0,$$
$$f(R) \equiv \ln\frac{2R}{1-R}; \quad g(R,T) \equiv \frac{5\kappa}{3k_BT}(1-R)^{2/3} - \frac{2C_2}{k_BT}(1-R). \tag{16}$$

We note that f(R) is a monotonically increasing, unbounded (at $R \to 0+$, and $R \to 1-$) function of R having one point of inflection at $R = 1/2$. However g(R,T) is a bounded function in the same domain. Hence g(R,T) must intersect f(R) at least once, i.e., eq.(16) must have at least one solution. In addition g(R,T) has a negative curvature and one maximum for $R \in [0,1]$. Thus there is a possibility of having more than one point of intersection with f(R) below a suitable temperature T_c.

In Fig. 1 we display some typical behaviours of f(R) and g(R,T). As shown, f(R), denoted by the solid line, approaches to $-\infty$ at R=0 and to ∞ at R=1. g(R,T) is a concave-downward curve. f(R) intersects the R axis at $R = 1/3$. g(R,T) intersects the R axis at two points: One is at R=1 which is independent of the values of the

parameters C_2, κ, and k_BT, and the second point of intersection depends on the ratio $\alpha \equiv 5\kappa/6C_2$ and importantly is independent of temperature T.

For low temperatures, the curves f(R) and g(R,T) may have three intersection points, as denoted by A,B, and C for the T=8 case. (Note that we use the convention of $k_B \equiv 1$.) It is readily checked that the middle intersection point, i.e. B, corresponds to a minimum of $\ln Q_G$ and hence it is not a physical solution. The intersection points A and C are the physical solutions. Note that g(R,T) is inversely proportional to the temperature. Hence as T increases, the right side of it sweeps down while its left side sweeps up, as shown in the figure. At some critical temperature T_c the curves f(R) and g(R,T_c) become tangent to each other. And afterwards the curves f(R) and g(R,T) have only one intersection point. g(R,T) eventually becomes a horizontal line as T approaches ∞, as indicated by the $T = \infty$ dotted line in the figure, and it obviously has just one intersection point with f(R).

In Fig. 2 we plot the solutions of eq.(16). As seen, we have two solutions, as indicated by points A and C of Fig. 1, for $T < T_c$, and for $T > T_c$ we have only one solution. This figure suggests that below T_c we have three regions, the dense(liquid-like) phase, the rare(gas-like) phase and the coexistence phase in between. The physical meaning of the above results may become clearer by examining the pressure-volume isotherms.

Before doing this, we should probably discuss the parameters C_2 amd κ which have entered into our calculations. To have an attractive nearest-neighbor interaction, we have $J_s > 0$ and $J_d < 0$. In this case C_2 is positive. The magnitude of J_s and J_d is probably comparable to the average potential energy in nuclear matter, which is about -40 MeV. Hence we have picked $C_2 = 125$ MeV, recalling that C_2 has been defined in eq.(9). The parameter κ may be estimated from the average kinetic energy given by the Fermi gas model. Assuming a lattice spacing of 1.5 fm and taking the nucleon mass as 940 MeV, κ is obtained as about 125 MeV. Hence as a general guideline, the parameters C_2 and κ should both be not too far from 125. The results of Figs.1 and 2, and 3 to be presented later, are all obtained with C_2=125 and κ=1.2αC_2 with a specially chosen α as discussed below.

Near the critical point, there is a subtle dependence of the solutions of eq.(16) on the ratio $\alpha \equiv \frac{5\kappa}{6C_2}$. As indicated by points A, B and C of Fig. 1, we have three intersection points below T_c. It is readily checked that by choosing $\alpha = (2/3)^{1/3}$, these three intersection points all merge together at the critical point. Then the phase diagram near T_c has the smooth shape as shown in Fig. 2. If one uses a slightly different ratio, the merging would generally take place in two steps, first involving two intersection points and then the third. This will lead to a phase diagram with a "cusp" shape near the critical point, which may seem to be rather unconventional. By intuition we feel that it is more reasonable to have a smooth phase boundary, and hence we have chosen the above α. With this α and C_2=125, we have κ=131.037, which has been used in obtaining the results presented in our Figs. 1 to 3.

For fixed T, the solutions of eq.(16) determines the R values where the grand partition function has a maximum contribution. In fact this maximum term is an overwhelmingly dominant one. (For finite lattices such as that with N=10^6, numerical simulation has shown that the magnitude of the maximum term is typically $\sim 10^{100}$ while for all the other terms it is $\sim 10^{20}$.) Hence the R values given by eq.(16) are just the average values of R, as denoted previously by $\bar{R}$, for the system at temperature T and λ=0. The $\bar{R}$ values for $\lambda \neq 0$ are given by the solution of eq.(15). Then the pressure at various densities and temperatures is given by

$$p(\bar{R}, T) \equiv \frac{k_B T}{N} \ln Q_G$$

$$= C_2(1-\bar{R})^2 - \kappa(1-\bar{R})^{5/3} - k_B T \bar{R} \ln(\frac{2\bar{R}}{1-\bar{R}}) - k_B T \ln(\frac{1-\bar{R}}{2}) + \lambda(1-\bar{R}). \quad (17)$$

Let us define the specific volume v as $(1-\bar{R})^{-1}$. Then we can calculate the p-v isotherms using eqs.(16) and (18). Our results are shown in Fig. 3.

Our figure seems to contain some interesting features. For a given temperature T the isotherm is obtained as a parametric plot of specific volume versus pressure with λ its generating parameter. For $T \geq T_c$ one gets a single smooth curve by varying λ. The boundary, drawn as a solid line at v$\simeq$ 1.5, corresponds to $\lambda = 0$. The isotherm to the

left of this boundary is obtained with positive λ, while to the right of this boundary the isotherm is obtained with negative λ. The critical temperature obtained is $T_c = 18.4$.

For T below T_c, it is of interest that no isotherms are obtained in the intermediate region, i.e. region I. For $\lambda < 0$, we get a gas-like isotherm starting from the high specific volume tail of the phase boundary. And for $\lambda > 0$ we get a liquid-like isotherm (very high compression modulus) starting from the lower specific volume edge of the phase boundary. The above is because when $T < T_c$, eq.(15) has no solutions in region I, the coexistence region. With the introduction of an infinitesimal λ the system chooses one of the two values of $\bar{R}$ admissible for the given $T < T_c$, depending on the sign of λ. This phenomena is reminisent of the spontaneous symmetry breaking in ferromagnetism.

There is another point which may be mentioned. As indicated in the figure, for a given isotherm the pressure at the liquid boundary and that at the gas boundary appear to be equivalent to each other, such as the apparent equivalence between the pressures of the T=12 isotherm at the two boundaries. We have examined this type of apparent equivalence, and have found that these two pressures are "exactly" equal to each other, within the accuracy of our computer. The structure of our calculated isotherms seems to strongly support that for $T < T_c$ our model gives a liquid phase, a gas phase and a coexistence phase with the boundary indicated by the solid line. And for $T > T_c$ the distinction between the liquid and gas phases disappears.

As a conclusion, let us state the following points. We have studied a simple lattice gas model for nuclear matter, where each lattice site can be either vacant or occupied, by one proton or by one neutron. A hamiltonian consisted of a nearest-neighbor interaction and a kinetic-energy term is assumed. The partition function is then calculated with the Bragg-William approximation. Some rather encouraging results have been obtained. A phase diagram consisting of liquid, gas and coexistance phases is obtained from our model. And the p-v isotherms given by our model are surprisingly similar to those given by the van der Waals theory, except for the difference that for $T < T_c$ our isotherms do not have the metastable states in the coexistence region. Hence with our model one does not need to determine the phase boundary by way of a Maxwell construction. The liquid-gas critical temperature obtained by us is $T_c = 18.4$ for sym-

metric nuclear matter, which is fairly close to the results given by earlier calculations [5, 4].

Comparing with earlier lattice gas models [12], a new ingredient of the present model is the introduction of the kinetic energy term. We recall that to have phase transitions we need the g(R,T) curve to have three intersection points with f(R) for $T < T_c$. Whether this happens or not clearly depends on α ($= 5\kappa/6C_2$). There is a wide range of values of α, for which this could happen. But if we don't have the kinetic energy term, then $\kappa = 0$ and $\alpha = 0$. And in this case the above requirement can not be met, and our model would have no phase transitions. Hence the inclusion of the kinetic energy term is important for our model. In fact in a previous paper [14] we have studied a lattice-gas model for nuclear matter, using the same lattice Hamiltonian as Eq.(5) but without the inclusion of the kinetic energy term; the results were clearly unsuccessful.

We have adopted a major approximation, the Braggs-Williams approximation, in the present work. The accuracy of this approximation remains to be investigated. More accurate calculations may be performed, using for example the Bethe-Peierls approximation [12], or Monte Carlo simulations which have been extensively in lattice-gauge and Ising-model calculations. With the Bragg-Williams approximation, the calculated phase boundary near the critical point can be either a smooth shape or a cusp shape. It should be of interest to see what would be the phase-boundary shape given by such more advanced methods.

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FIGURE CAPTIONS

Fig.1 Graphical solution of eq.(16).

Fig.2 Nuclear matter phase diagram given by our model.

Fig.3 Nuclear matter p-v isotherms.